

Developing Dynamical Mean-Field Methods for Actinide Materials Simulation at AWE

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Electronic structure simulations for actinide materials are complicated by the propensity of the 5f electrons to form strongly correlated ground states. To model these states accurately, a combination of efficient density functional theory (DFT) and many-body methods, chiefly Dynamical Mean-Field Theory (DMFT) is required. Several questions of industrial importance require models to describe the influence of local perturbations on the electronic structure. Examples include the surface chemistry of a solid, or predicting structural relaxations due to a lattice defect or dislocation. To simulate these effects in conjunction with strong correlations requires scalable and accurate DMFT implementations that can work with large unit cells, even when neglecting non-local correlations. Ongoing work to develop such a capability at AWE is presented.